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Multiscale modeling of the deformation of Ta*

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We are developing constitutive models for the deformation of Ta polycrystals using the multiscale modeling approach. This approach embodies modeling at three distinct length scales the meso-, micro-, and atomistic length scales. Ultimately at the mesoscale, a virtual test sample composed of hundreds of grains will be "deformed" along prescribed strain paths to produce an anisotropic yield surface that evolves with strain as the microstructure evolves. The inputs for the mesoscale simulations, yield point and hardening law, come from simulations at the microscale where dislocations are modeled discretely. The rules for dislocation motion and interaction come from simulations at the atomic length scale. Successful multiscale material models have the potential to be predictive rather than only descriptive.

In this presentation, we describe results of our multiscale model for the deformation of a bicrystal. This model operates at the mesoscale and uses input from the atomic and micro length scales. Results for crystal rotation (as a function of location relative to the grain boundary) as a function of strain will be compared with observations of a bicrystal deformed experimentally.

Key: Multiscale modeling, strain-gradient crystal plasticity, microscale simulations, atomistic simulations

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